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MAH-3 Code: Mixed Cells and Markers to Reconstruct Interfaces

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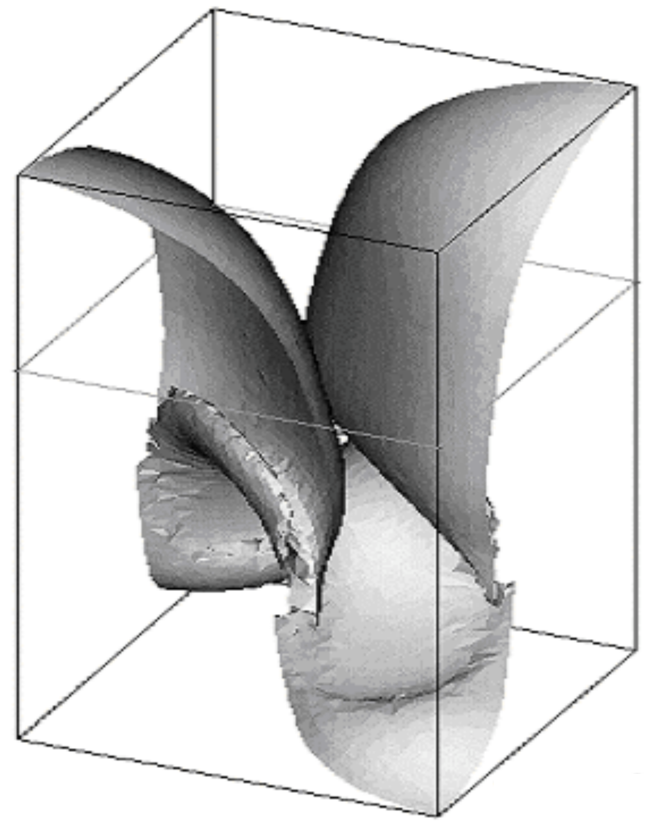
MAH-3 [1, 2] code simulates nonstationary 3D hydrodynamic multi-component flows with strongly distorted interfaces.

Following from a priori information, the system to be simulated is presented by a set of computational domains.

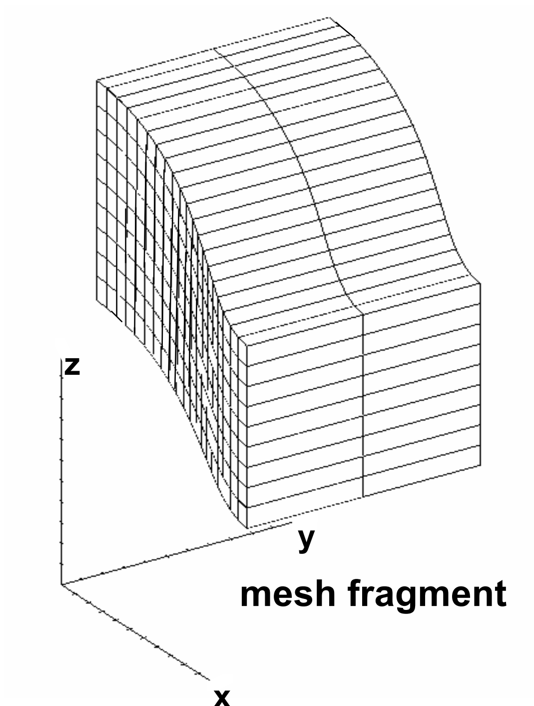
In each domain, an unstructured hexahedral mesh is used.



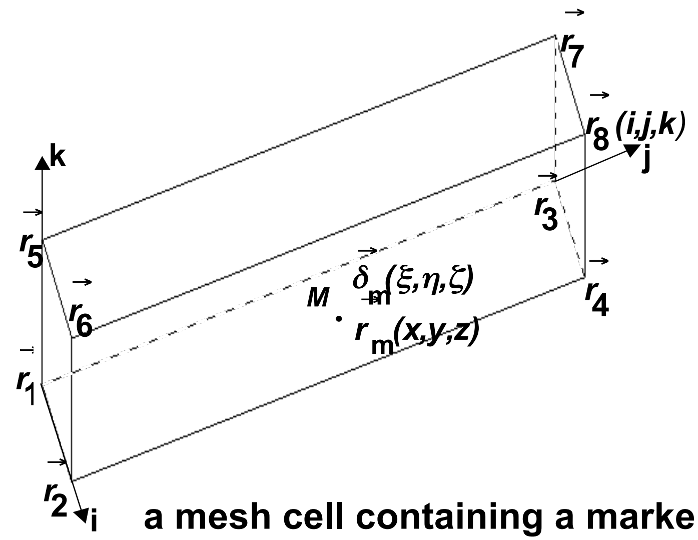
1. *Anuchina N.N., Volkov V.J., Gordeychuk V.A., Es'kov N.S., Ilytina O.S., Kozurev O.M. Numerical simulation of Rayleigh-Taylor and Richtmyer-Meshkov instability using MAX-3 code. Journal of Computational and Applied Mathematics, vol. 168 (2004), pp. 11-20.*

2. *Volkov V.I., Gordeychuk V.A., Es'kov N.S., Kozyrev O.M. Numerical simulation by the MAH-3 code of the interfaces using an unstructured mesh of markers. Laser and Particle Beams,18 (2000), pp.197*

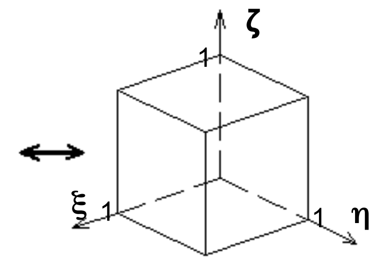
Structured hexahedral mesh



mesh fragment



a mesh cell containing a marker in physical space (x,y,z)



unit cube in parametric space (ξ,η,ζ)

The relation between $\vec{r}_m(x,y,z)$ **and** (ξ,η,ζ)**:**

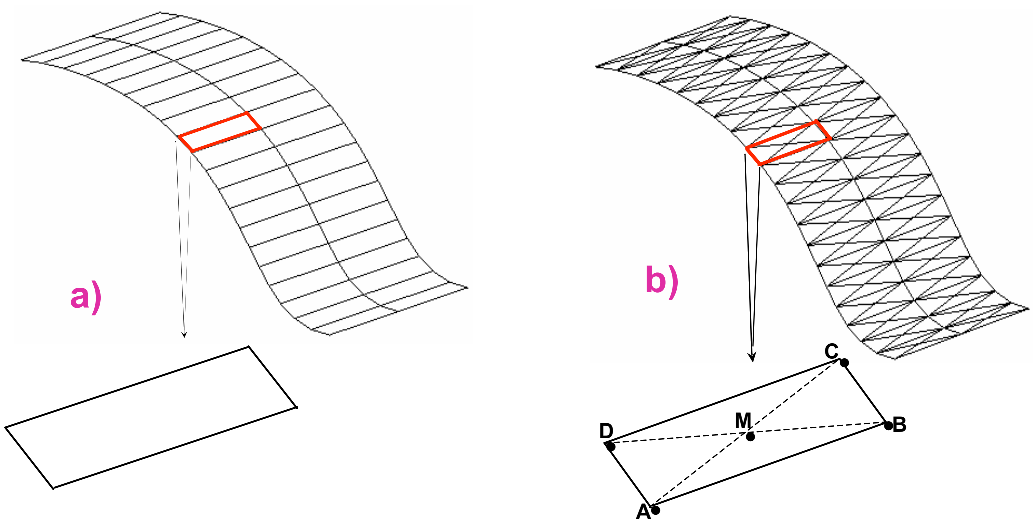
$$\vec{r}_m(x,y,z) = (1-\xi)(1-\eta)(1-\zeta)\vec{r}_1 + \xi(1-\eta)(1-\zeta)\vec{r}_2 + (1-\xi)\eta(1-\zeta)\vec{r}_3 + \xi\eta(1-\zeta)\vec{r}_4 +$$

$$(1-\xi)(1-\eta)\zeta\vec{r}_5 + \xi(1-\eta)\zeta\vec{r}_6 + (1-\xi)\eta\zeta\vec{r}_7 + \xi\eta\zeta\vec{r}_8 \quad \Rightarrow \quad \vec{\delta}_{\mathbf{m}}(\xi,\eta,\zeta);$$

$$\text{where: } \quad 0 \le \xi \le 1, \quad 0 \le \eta \le 1, \quad 0 \le \zeta \le 1$$

In detailed study of the contact boundary evolution we turn to the description of the contact boundary by means of combined cells and Lagrange triangular mesh of markers, which is not connected with the mobile Euler mesh of numerical integration area;

Creation of initial triangular mesh of markers



Mapping of an initial triangular mesh of markers at the contact boundary (and a zoomed face):

a) prior to initialization;

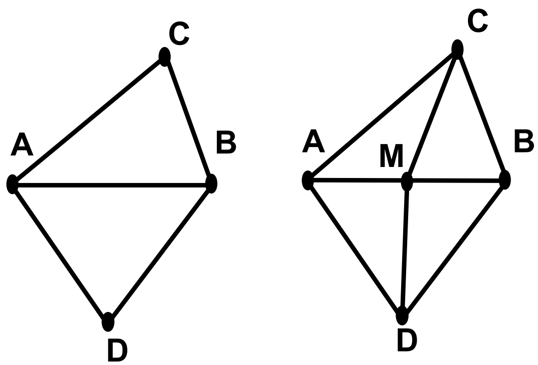
b) after initialization.

A triangular mesh is used for the description of the contact surface in a 3D space. Each nod of the mesh is a marker, and the marker motion is defined by the velocity field of the medium.

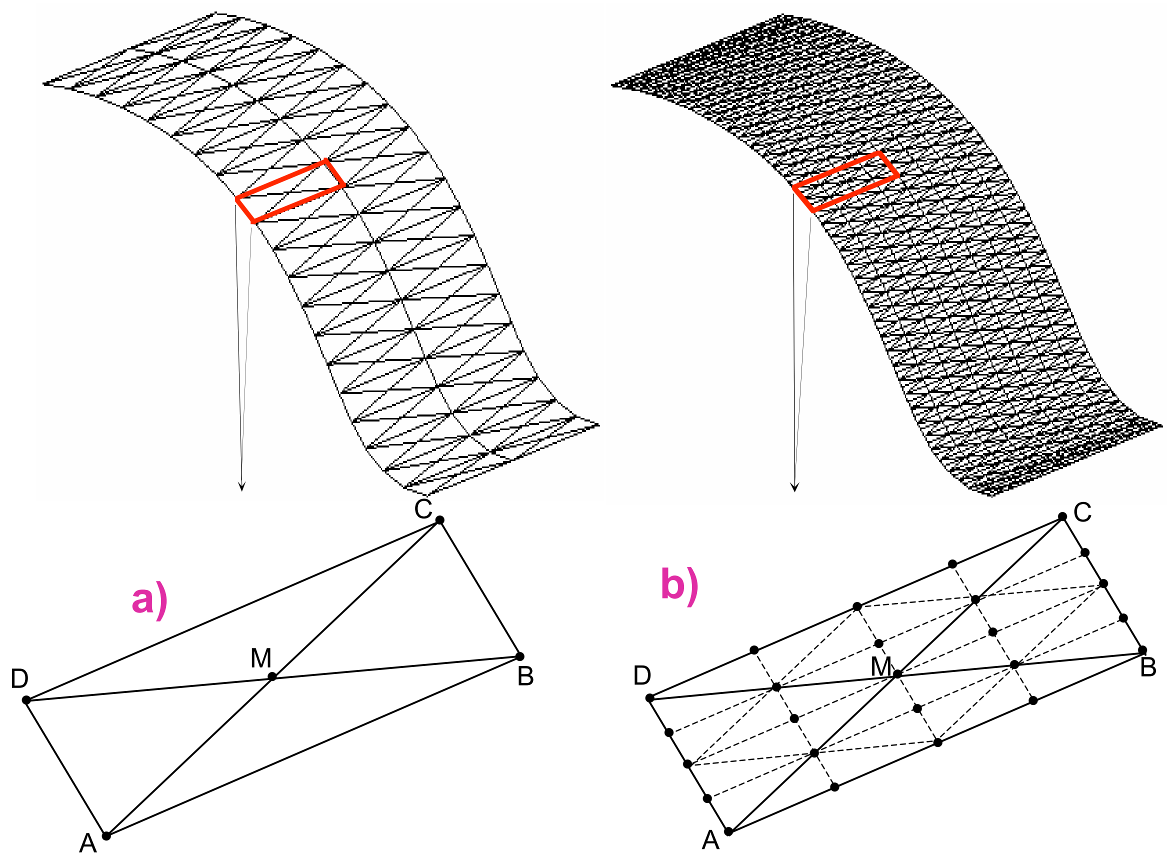
The edges of the triangles define the relation between the markers at the contact surface, and this stipulates the mesh topology

Required quality of the marker mesh is supported for the account:
- addition of new markers;
- re-mapping of the marker triangular mesh.

Addition of the marker

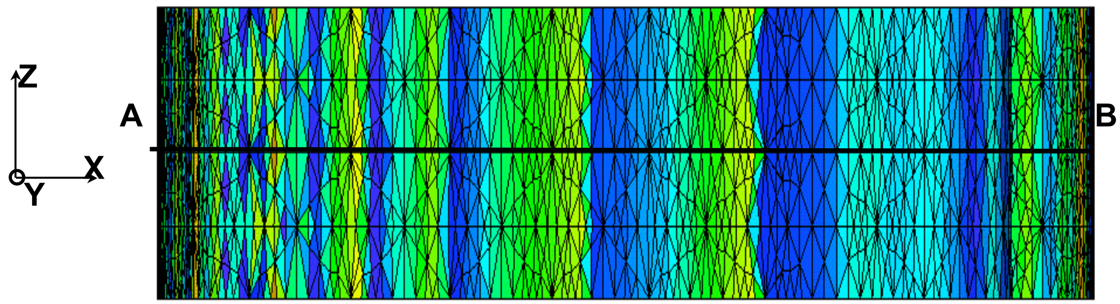


Addition of a new marker M

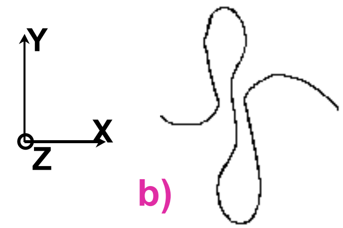


Example of adding new markers (and a zoomed face):
a) prior to addition;
b) after addition.

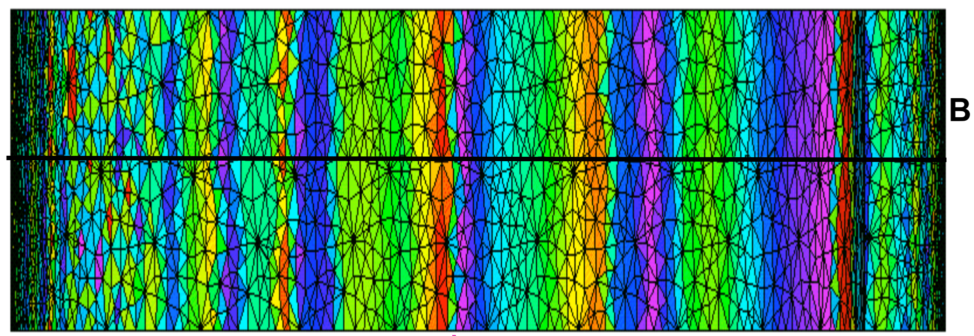
Conservation of symmetry in 2D calculations



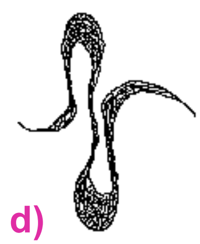
a)



b)



c)

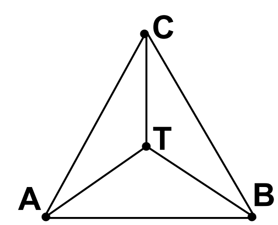


d)

3D view mesh of markers: a), c) – Y = const and b), d) – Z = const:

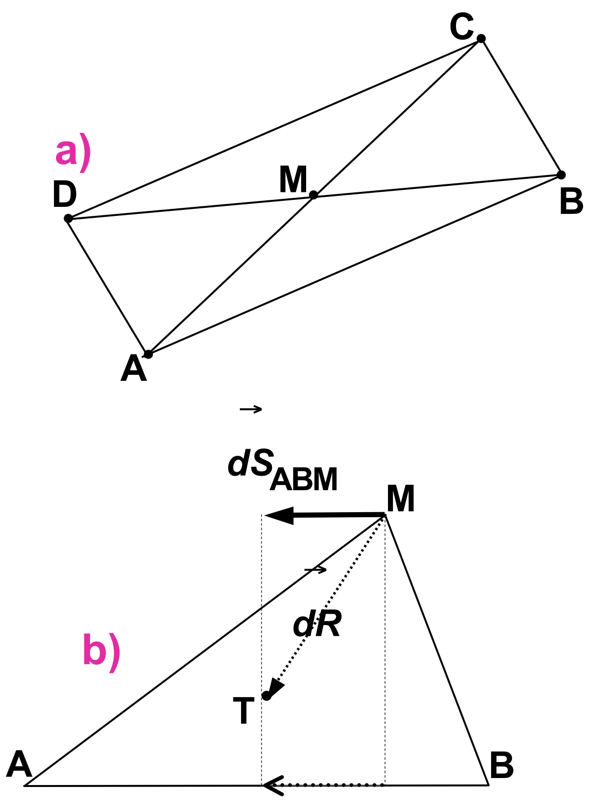
a), b) the requirement of symmetry <u>is met;</u>

c), d) the requirement of symmetry <u>is not met.</u>

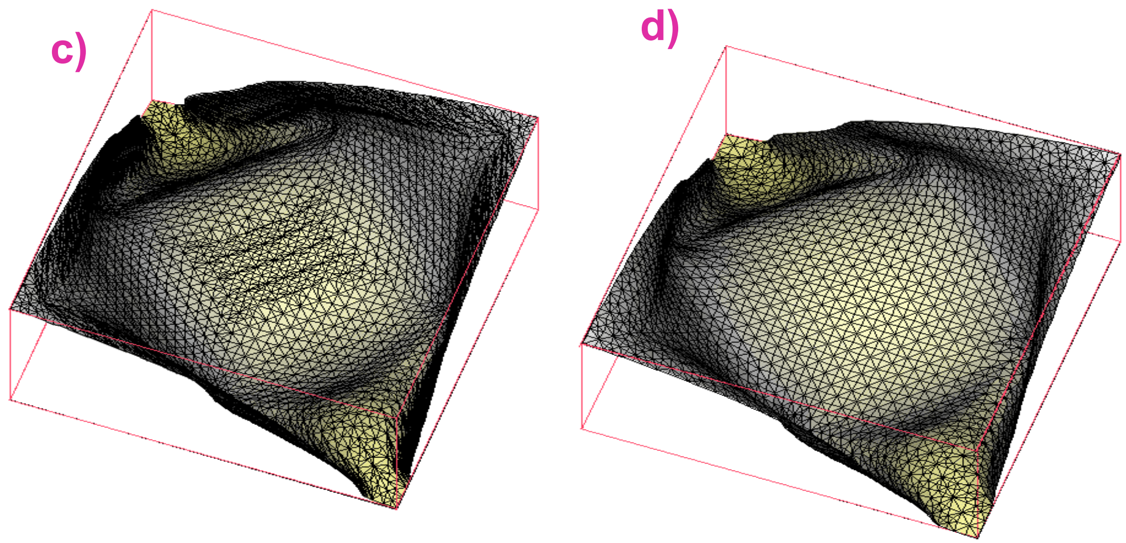


Resolution of the “conflict”

Triangular marker mesh remapping

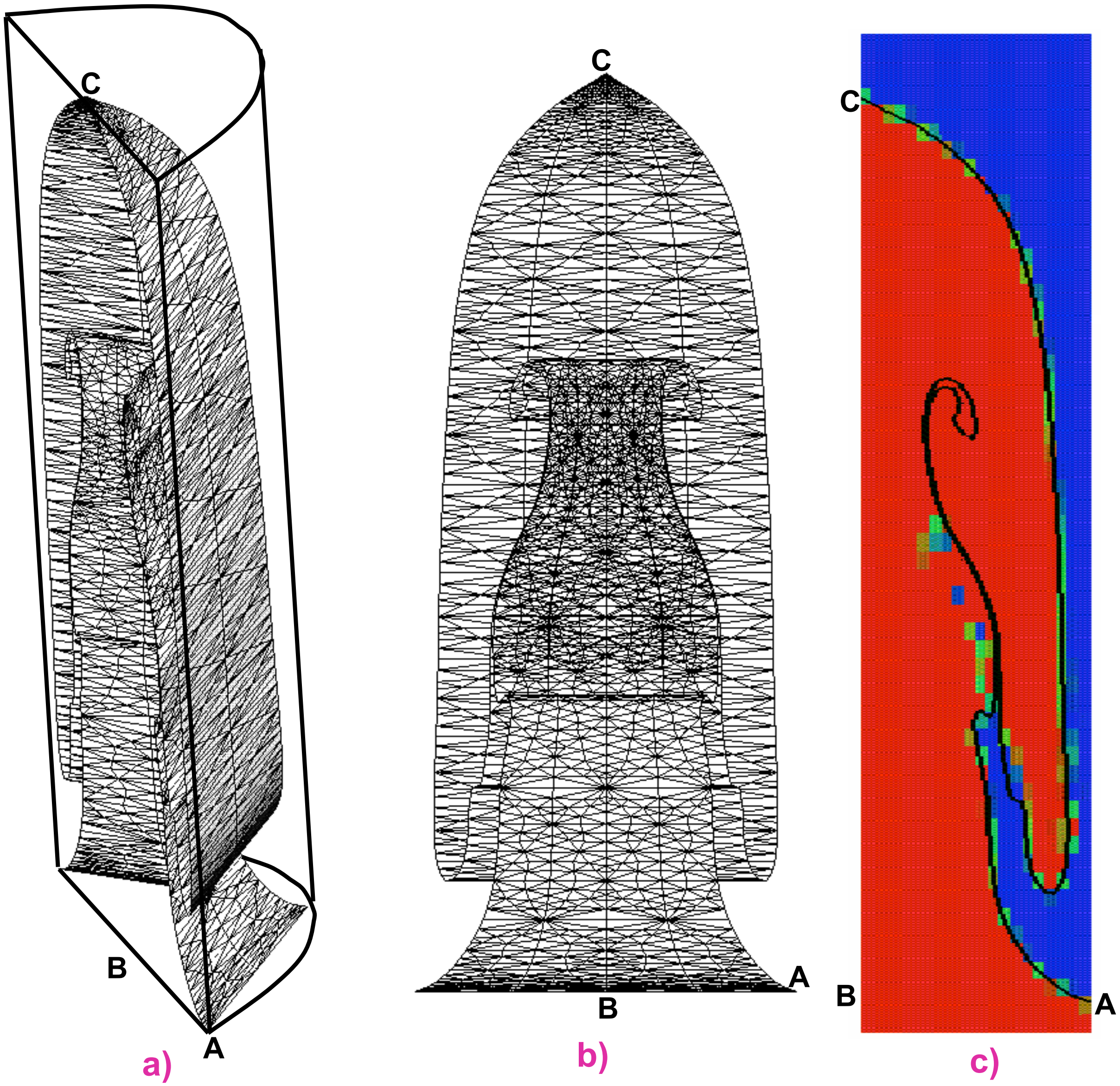


Marker M remapping :
a) Marker M and all triangles having M as a vertex;
b) M displacement vector $d\vec{S}_{ABM}$ obtained from triangle ABM



Unstructured triangular mesh on the contact surface:
c) No remapping (6,500 markers);
d) Remapping (2,500 markers)

Rayleigh-Taylor instability. Evolution of regular perturbation in 2D cylindrical case (ρ_2/ρ_1=10).
The interface is represented by a triangular mesh of markers.

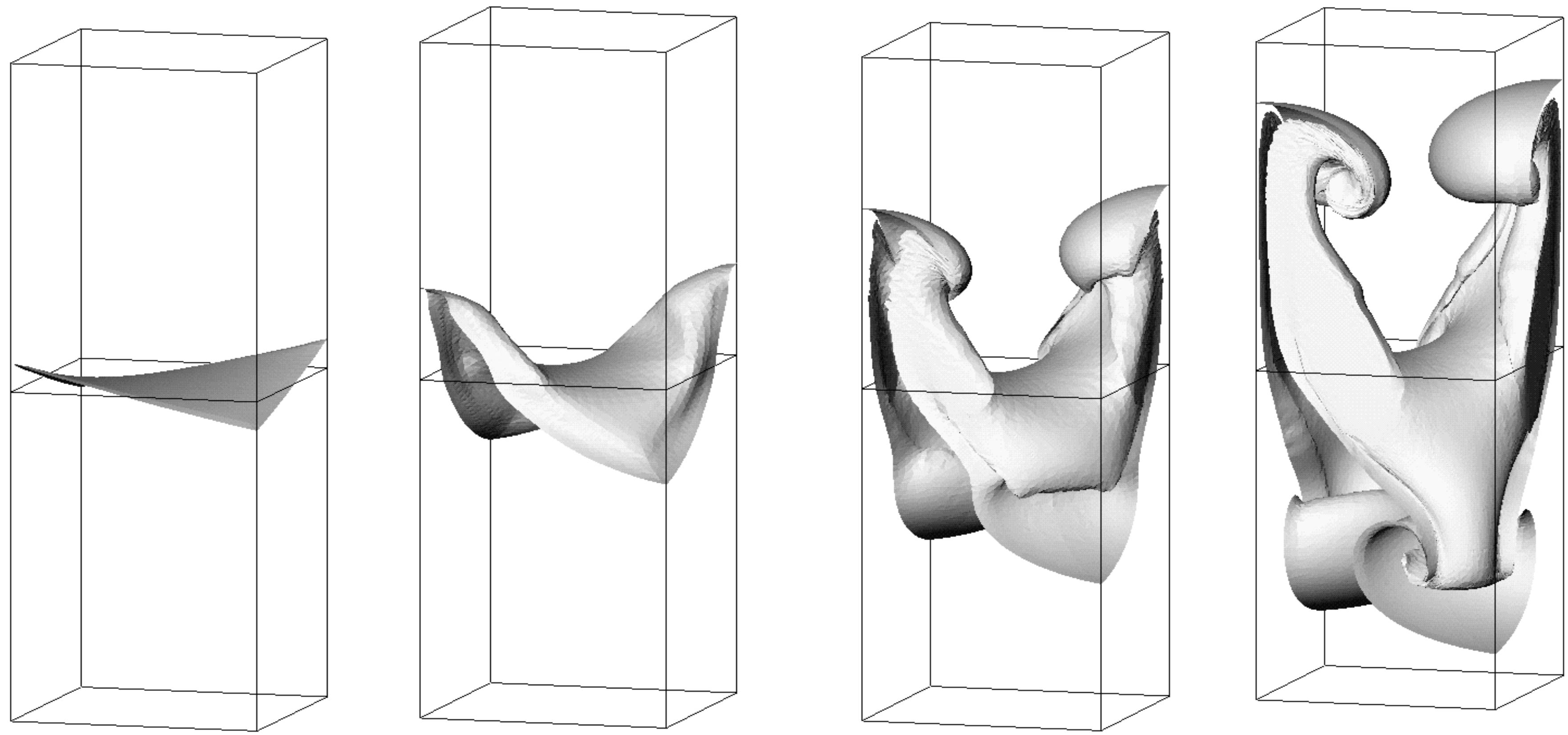


a) **3D interface covered with an unstructured triangle mesh;**

b) **Front view of the interface (full markers mesh). It demonstrates preservation of 2D-quality of the mesh of markers;**

c) **2D interface presented by the mesh of markers as in b) with the density field as a background. An agreement is shown between positions of the markers and the mixed cells**

Rayleigh-Taylor instability (ρ2 /ρ1=1.1): growth of perturbations at the interface in 3D case (at different times). The interface is represented by the triangular markers mesh.



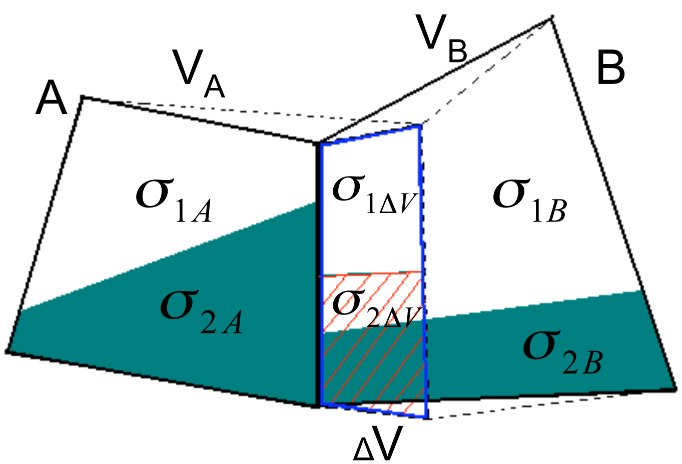
time=1.2 **time=1.7** **time=2.2** **time=2.7**

One of the basic requirements: two neighbor markers must be either in one cell or in neighbor cells.

For each marker, not only coordinates are stored, but also data on the difference cell where the marker is added and on materials at different sides of the interface to which the marker belongs.

This **marker information** is quite sufficient to determine **the “new” matter composition** in each difference cell for the next step, **before treating convective flows**.

With these data we can appropriately correct convective flows using **markers and concentrations**.



The flow of fluids 1 and 2 in the cells A and B:

«- -» - after Lagrangian phase
«—» - new mesh

$$V_A' = V_A + \Delta V$$
$$V_B' = V_B - \Delta V$$

$\sigma_{1\Delta V}$? $\sigma_{2\Delta V}$?

Concentrations

If $\sigma_{1A} = 1$, $\sigma_{2A} = 0$: $\sigma_{1\Delta V} = 1$, $\sigma_{2\Delta V} = 0$.

...

If $\sigma_{1A} > 0$, $\sigma_{2A} > 0$, $\sigma_{1B} > 0$, $\sigma_{2B} > 0$:

$\sigma_{1\Delta V} = ½(\sigma_{1A} + \sigma_{1B})$; $\sigma_{2\Delta V} = ½(\sigma_{2A} + \sigma_{2B})$.

Markers and concentrations

If material 1 is absent in the new composition in B but present in A, then $\sigma_{1\Delta V} = 1$, $\sigma_{2\Delta V} = 0$.

...

If materials 1 and 2 are present in B, then similar to the concentration method.

Test problems:

1. **Homogeneous translational motion:** 2D and 3D tests to check material translation on a Eulerian mesh both along mesh lines and at an angle. One fluid is background and the other is shaped: for 2D, a square or circle (in a cross-section in the third direction); for 3D: a cube or sphere. These tests are used to check numerical methods for ability to hold interface shapes.

2. **Heterogeneous translational motion:** very simple and effective 2D and 3D tests to adjust fluids flows on a Eulerian mesh. Physical processes are not involved since at any time the velocity of any point in the system is a function of only space and time.

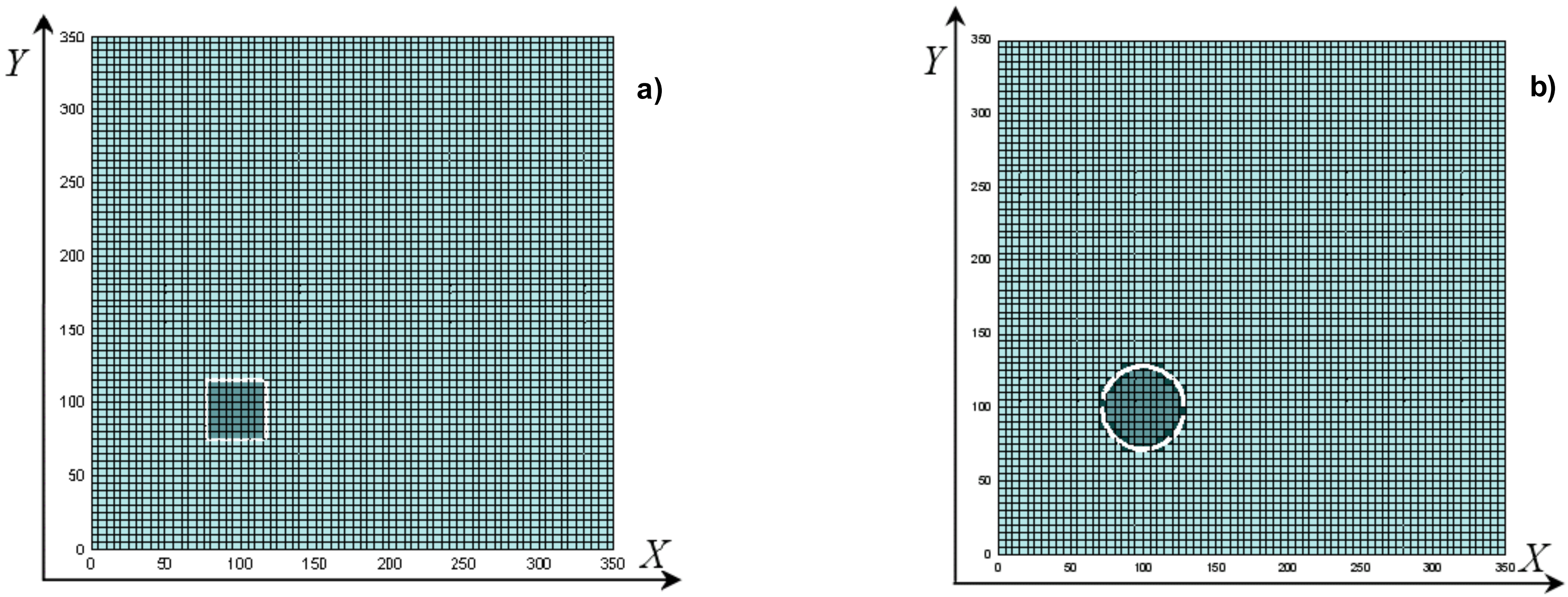
All test problems have “exact” solutions.

Purpose:

1. Compare two interface reconstructing algorithms based on
   - the method of concentrations; and
   - the method of markers (i.e., interface reconstruction with an unstructured mesh of markers which move in accord with convective flow calculation); and
2. Demonstrate the capabilities of the two methods.

Homogeneous translational motion

Two incompressible non-viscous non-heat-conducting materials move at a constant velocity against a Eulerian mesh.



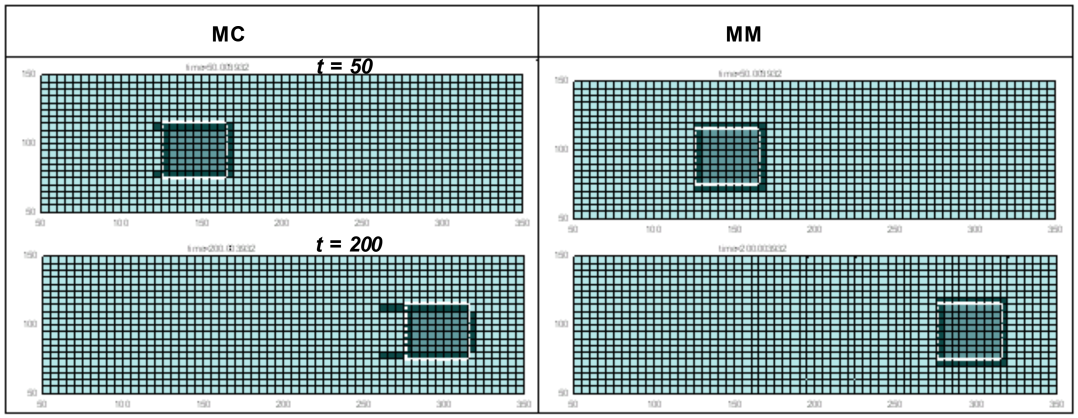
Initial configurations

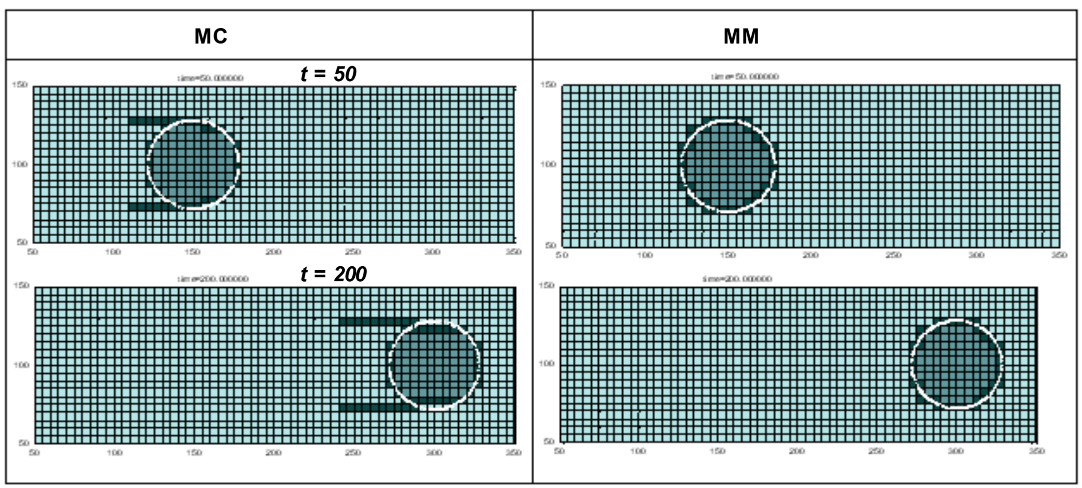
a) square or cube; b) circle or sphere

The marker mesh is shown in white.

2D calculation

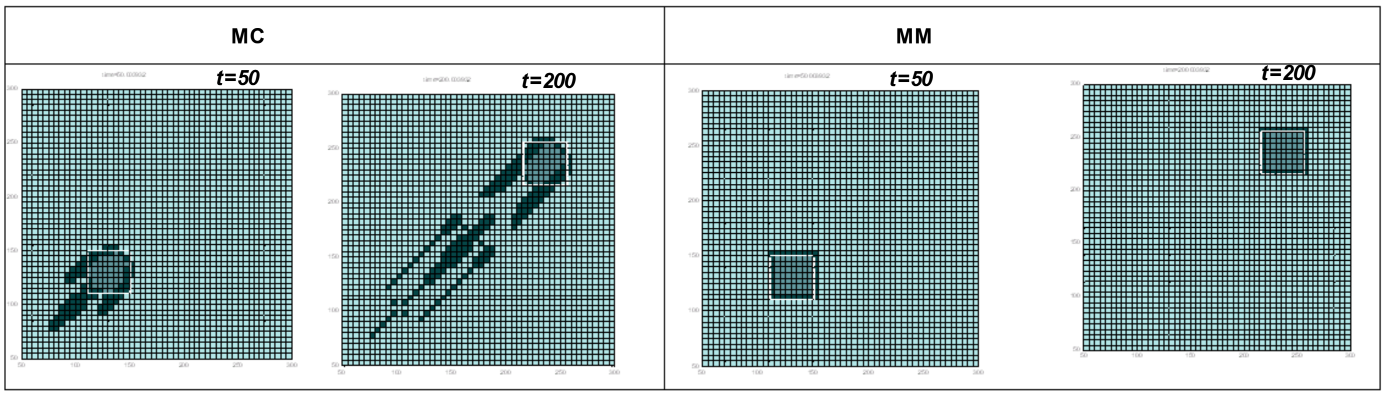
- Calculation domain: a brick 350x350x15 divided into cubic cells
- Cell size: 70x70x3
- Fluid 2 is shaped as a cylinder generated by 1) a square 40x40;   2) a circle R=25.
- Free flow on boundaries along *X* and the others are rigid walls
- No density difference
- Initial velocity: [1, 0, 0].
- Time step: 0.1, i.e. $\left|\vec{u}\right|\tau/h \approx 0.01$
- EOS: P = 0

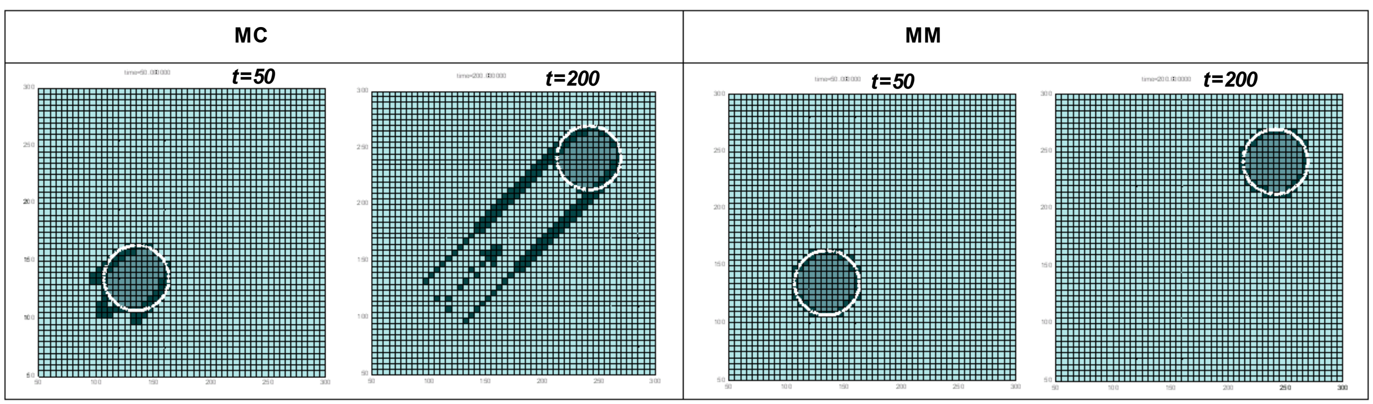




2D calculation

- Computational domain: a brick 350x350x15 divided into cubic cells
- Number of cells: 70x70x3
- Fluid 2 is shaped as a cylinder generated by 1) a square 40x40;   2) a circle R=25.
- Free flow on boundaries along *X* and Y, and the other boundaries are rigid walls
- No density difference
- Initial velocities: $[\sqrt{2}/2, \sqrt{2}/2, 0]$
- Time step: 0.1, i.e., $|\vec{u}|\tau/h \approx 0.01$
- EOS: P = 0.

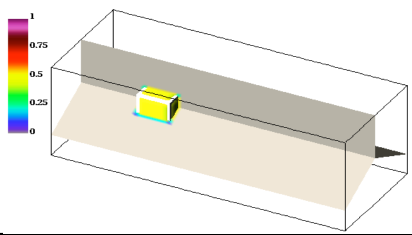
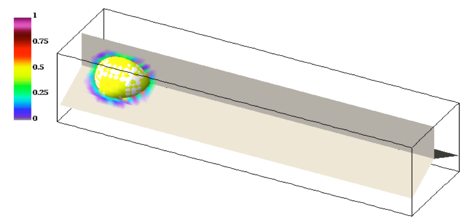
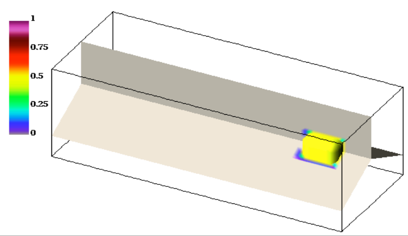
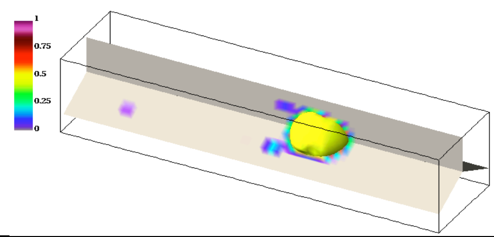
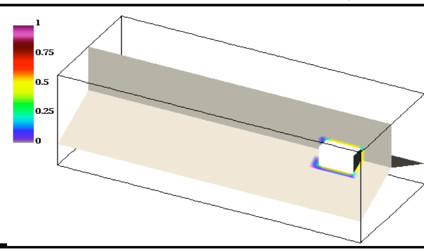
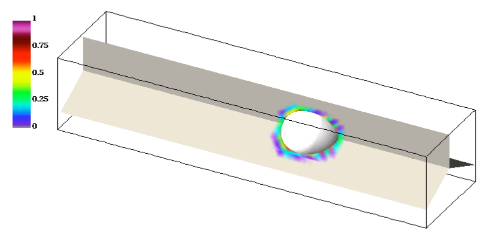




3D calculations

- Computational domain is a brick of sizes 1)350x140x140 and 2) 2x0.5x0.5, divided into cubic cells
- Number of cells: 1) 70x28x28 and 2) 64x16x16
- Fluid 2: 1) a cube of size 40x40x40 (8x8x8 cells)
  2) a sphere of radius 0.15, centered at (0.25, 0.25, 0.25)
- Free flow on boundaries along *X;* others are rigid walls
- Density ratio: 1/10
- Initial velocity: [1, 0, 0].
- Time step: 1) 0.001÷0.1 , i.e., $|\vec{u}|\tau/h \approx 0.0001 \div 0.01$ 2) 0.0001÷0.0045, i.e., $|\vec{u}|\tau/h \approx 0.002 \div 0.08$
- EOS: P = 0.

Cube and sphere volume fractions along mesh lines on three section of the computational domain
The marker mesh is shown in white and the isosurface for $\sigma = 0.43$ is in yellow.

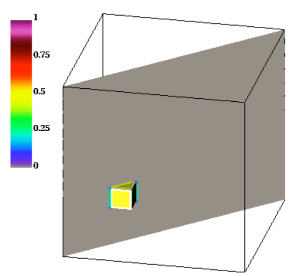
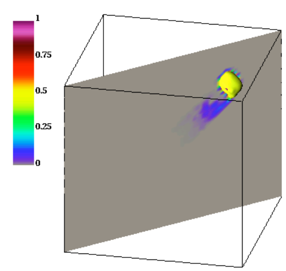
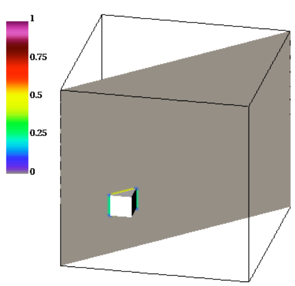
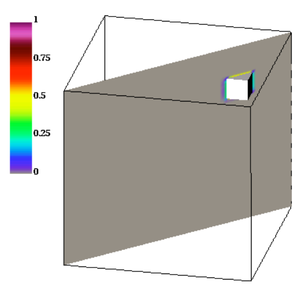
Problem	Cube translation along mesh lines	Sphere translation along mesh lines
MC, MM	 $t = 0$	 $t = 0$
MC	 $t = 200$	 $t = 1$
MM	 $t = 200$	 $t = 1$

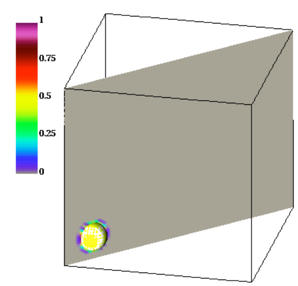
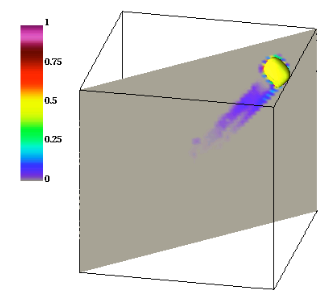
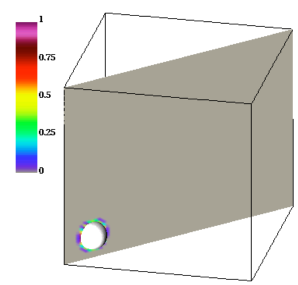
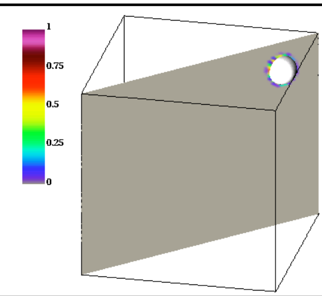
3D calculation

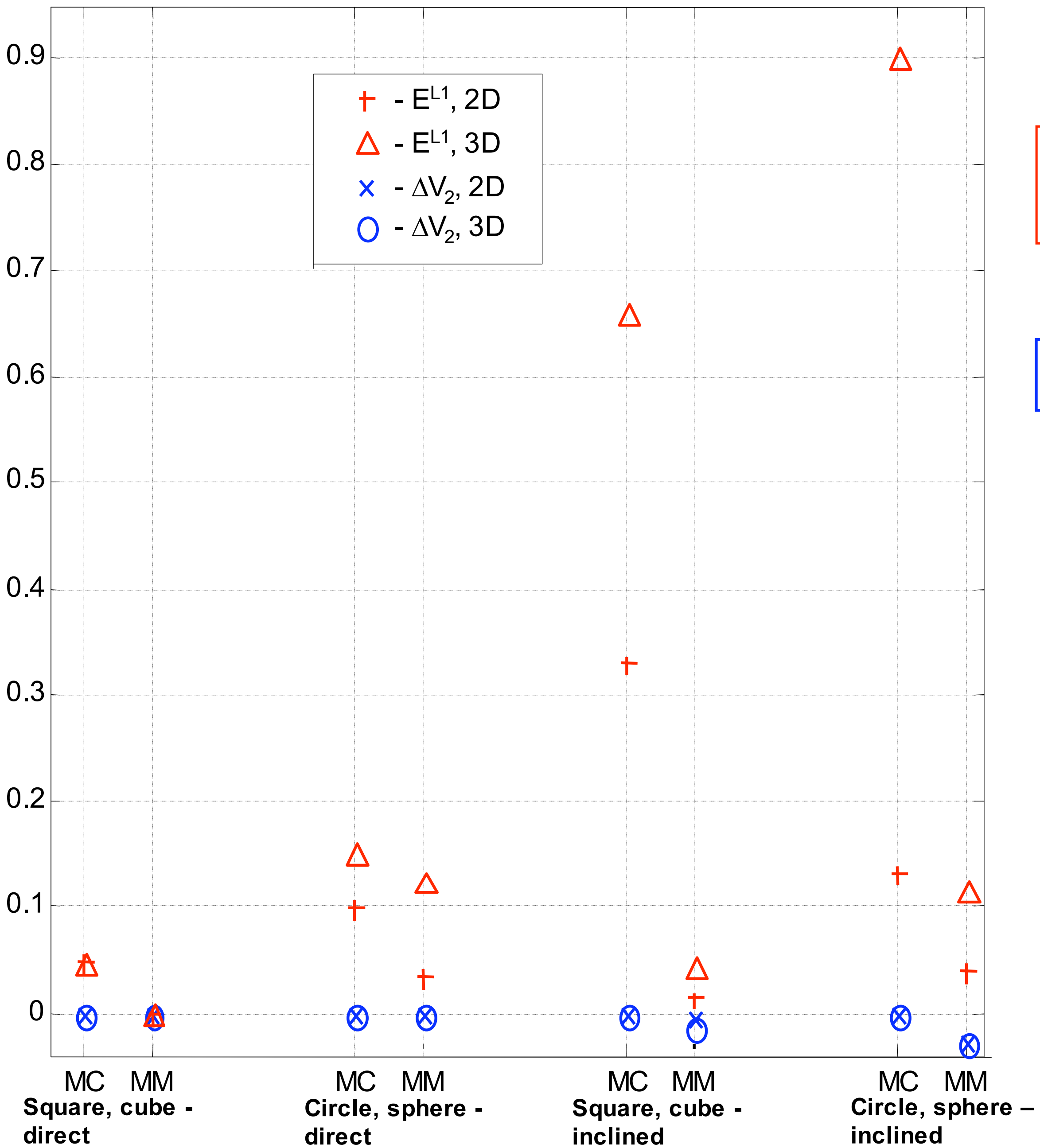
- Computational domain: a brick of sizes 1) 350x350x350 and 2) 2x2x2, divided into cubic cells
- Number of cells: 1) 70x70x70; 2) 64x64x64
- Fluid 2:
  1) a cube of size 40x40x40 (8x8x8 cells)
  2) a sphere of radius 0.15, centered at (0.25, 0.25, 0.25)
- Free flows on boundaries
- Density ratio: 1/10.
- Initial velocity: [0.57735, 0.57735, 0.57735].
- Time step: 1) 0.001÷0.1, i.e., $|\vec{u}|\tau/h \approx 0.0001 \div 0.01$ 2) 0.0001÷0.0045, i.e., $|\vec{u}|\tau/h \approx 0.002 \div 0.08$
- EOS: P = 0

Cube and sphere volume fractions on a diagonal section of the computational domain (inclined flow)

Interface: the marker mesh is shown in white and the isosurface for $\alpha = 0.43$ in yellow.

	$t = 0$	$t = 300$
MC		
MM		

	$t = 0.0$	$t = 2.5$
MC		
MM		



Error in σ_2:

$$E^{L_1} = \frac{1}{V_2^{exact}} \sum_{grid} V_{i,j,k} \left| \sigma_{2i,j,k}^{\text{computed}} - \sigma_{2i,j,k}^{\text{exact}} \right|$$

Volume delta:

$$\Delta V_2 = (V_2^{\text{computed}} - V_2^{\text{exact}}) / V_2^{\text{exact}}$$

Heterogeneous translational motion

Rider W.J. , Kothe D.B. “Reconstructing Volume Tracking”, Jornal of Computational Physics 141, 112-152 (1998)

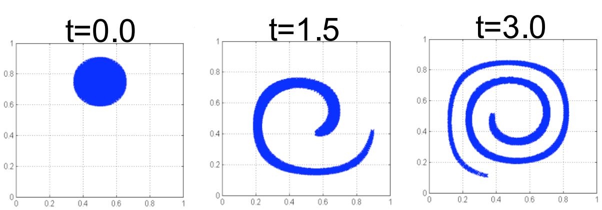
Setting of the 2D calculations:

- **Calculation domain – unit cube 1x1x1, divided into bricks**
  Number of bricks: 1) 32x32x2   2) 64x64x2   3) 128x128x2
- **Time step: 1) 0.004   2) 0.002   3) 0.001**
- **The cube is filled with fluid 1. A cylinder filled with fluid 2 is inside the cube. The cylinder is generated round the Z axis; its base is a circle of radius 0.15, centered at (0.5, 0.75).**
  Material distribution in mesh cells was defined by concentrations.
- **Studied is cylinder deformation in the velocity field:**

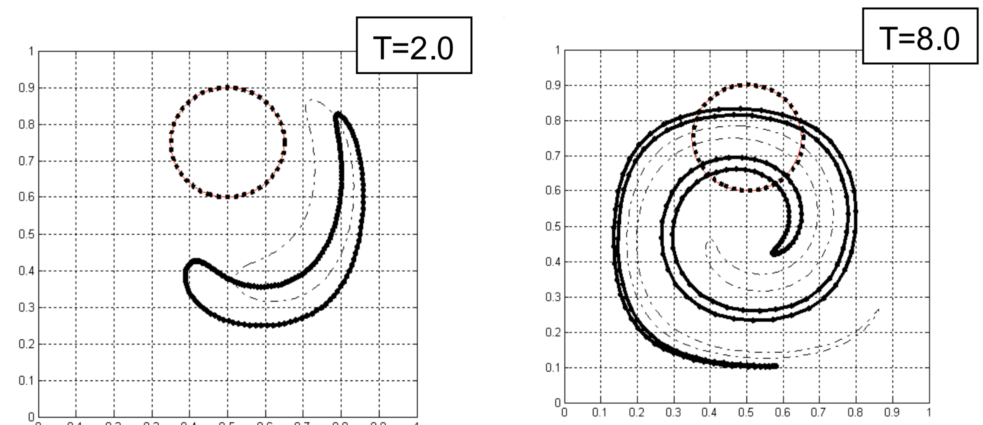
$$u = -\left(\sin(\pi x)\right)^2 \sin(2\pi y) \qquad\qquad u = -\sin^2(\pi x)\sin(2\pi y)\cos(\pi t / T)$$
$$v = \left(\sin(\pi y)\right)^2 \sin(2\pi x) \qquad \textbf{or} \qquad v = \sin^2(\pi y)\sin(2\pi x)\cos(\pi t / T)$$
$$w = 0 \qquad\qquad w = 0$$

Time–reversed flow fields

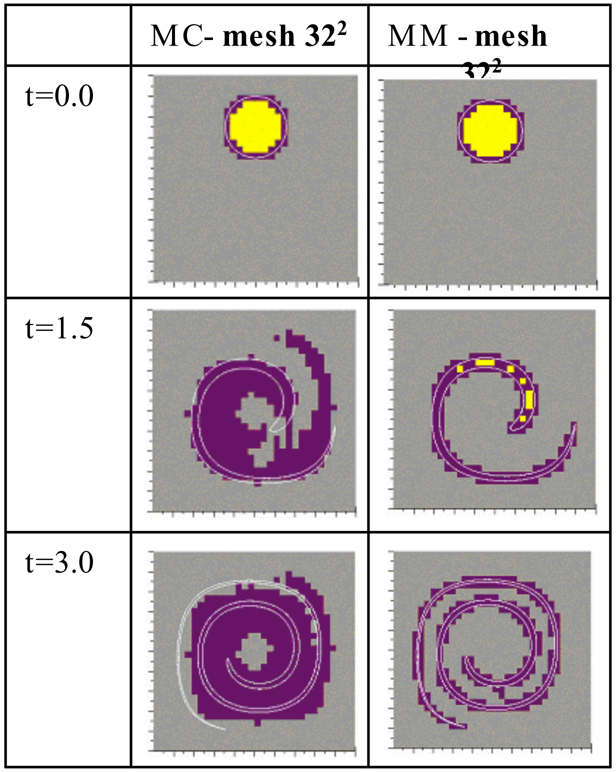
Stationary velocity field



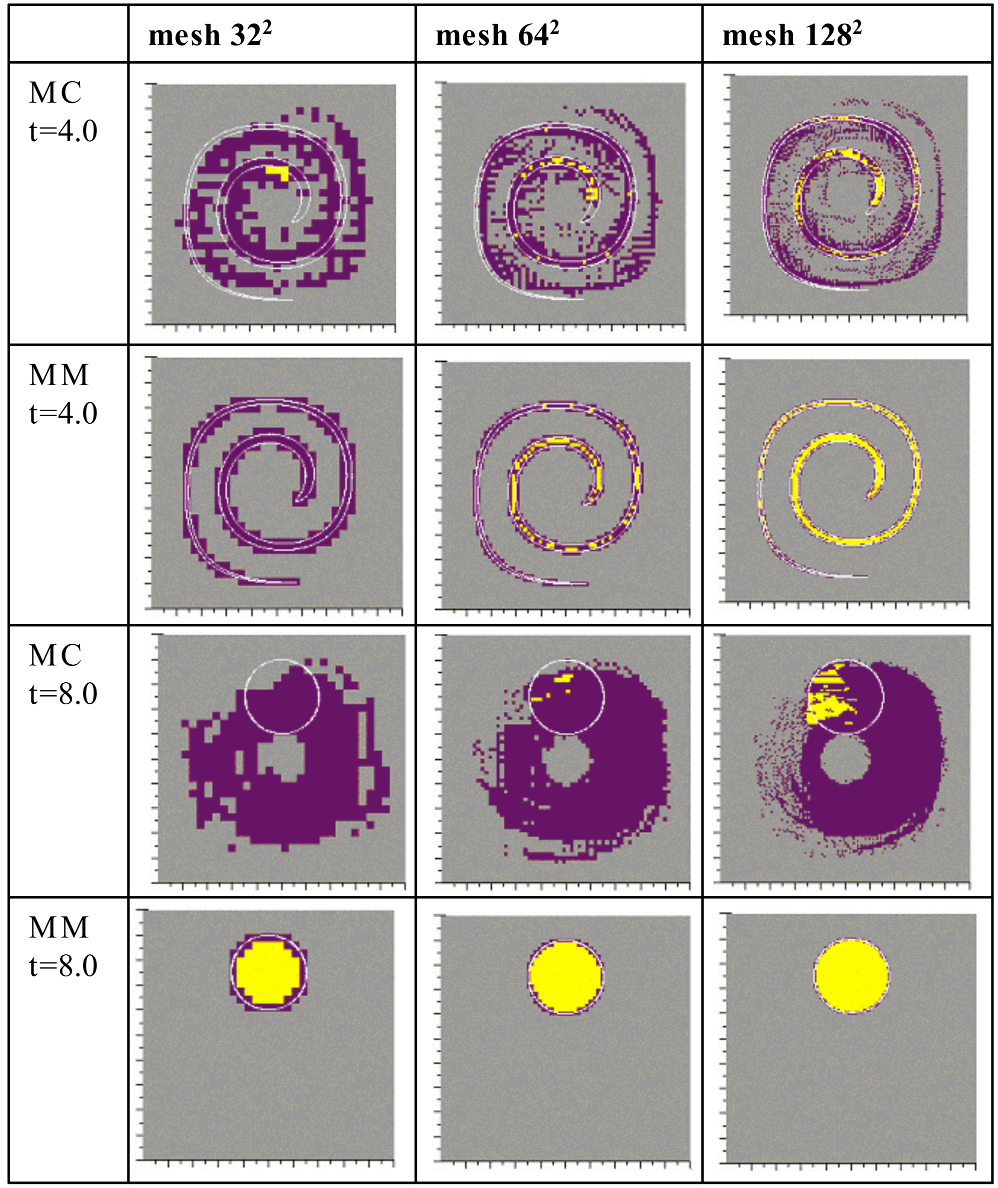
“Exact” solution (marked particles): the flow does nor reverse with time



“Exact” solution (the flow reverses with time) at times:
t=0 (points); t=0.25T and t=0.75T (dashes); t=0.5T (bold)



Materials and their interface (white) at t=0.0, t=1.5, and t=3.0 in the <u>constant velocity field</u>. MC – method of concentrations; MM – method of markers



Materials and their interface (white) at t=4.0 and t=8.0 in the <u>time-reversed velocity filed, period T=8.0</u> on different meshes: MC – method of concentrations; MM – method of markers

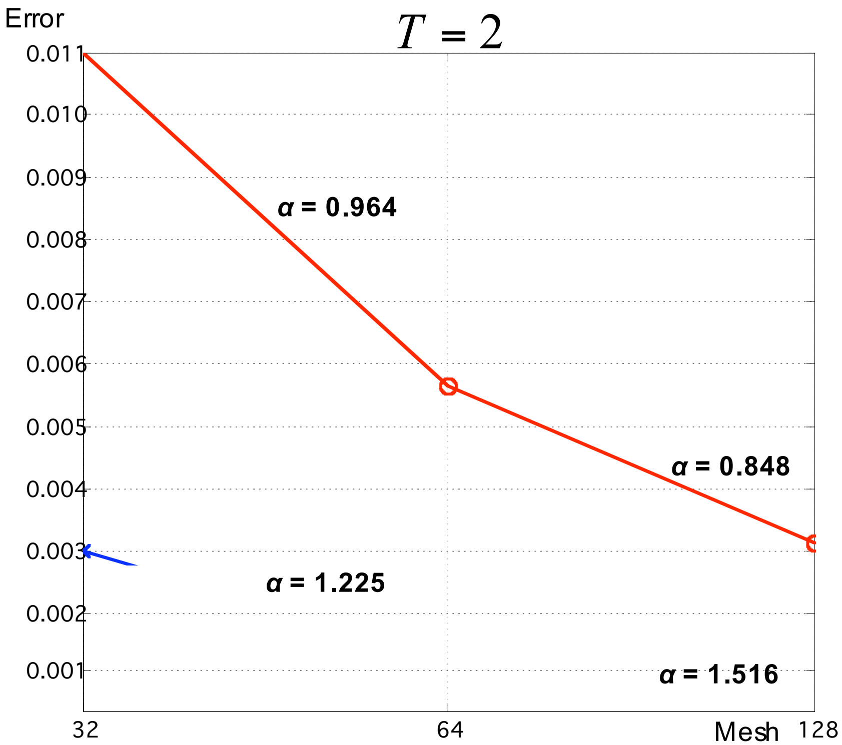
Errors in 2D calculations on the cylinder in a time-reversible flow fields, period *T* *(convergence tests)*

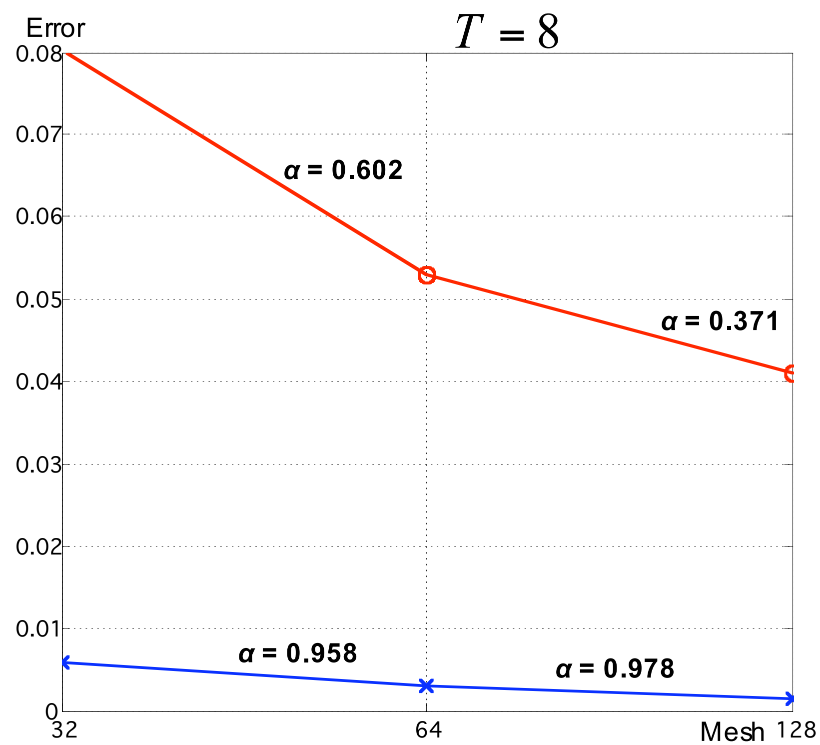
L_1 errors norms:

$$E^{L_1} = \sum_{grid,k=fix} V_{i,j,k} \left| \sigma_{2i,j,k}^{\text{computed}} - \sigma_{2i,j,k}^{\text{exact}} \right|$$

Convergence exponent α:

Let $q_1 = \text{£} h_1^{\alpha}$ *and* $q_2 = \text{£} h_2^{\alpha}$,
then $\alpha = \mathbf{log}(q_1/q_2)/\mathbf{log}(h_1/h_2)$,
where q - **L_1** errors **norms**, h - mesh spacing





L_1 convergence rates:
concentrations ~0.9
markers ~1.35

L_1 convergence rates:
concentrations ~0.5
markers ~0.97

3D calculation

- **Computational domain: a cube 1x1x1, divided into brick cells; number of cells: 32x32x32**

- **The cube is filled with material 1. A sphere filled with a liquid (material 2) is put inside the cube. The sphere has a radius of 0.15 and is centered at (0.5, 0.75, 0.75). Material distribution in mesh cells was defined by concentrations.**

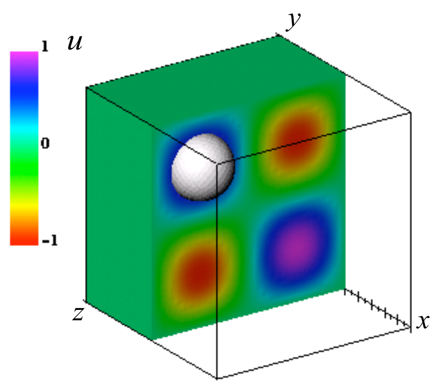
- **Constant time step: 0.004**

- **Studied is sphere deformation in a velocity field; velocity components:**

$$u = \left(\sin(\pi x)\right)^2 \sin(2\pi y)\sin(2\pi z)\cos(\pi t/T)$$

$$v = \left(\sin(\pi y)\right)^2 \sin(2\pi x)\sin(2\pi z)\cos(\pi t/T)$$

$$w = -2\left(\sin(\pi z)\right)^2 \sin(2\pi x)\sin(2\pi y)\cos(\pi t/T).$$



Velocity component distribution along the section x=0.5 and sphere at the initial time

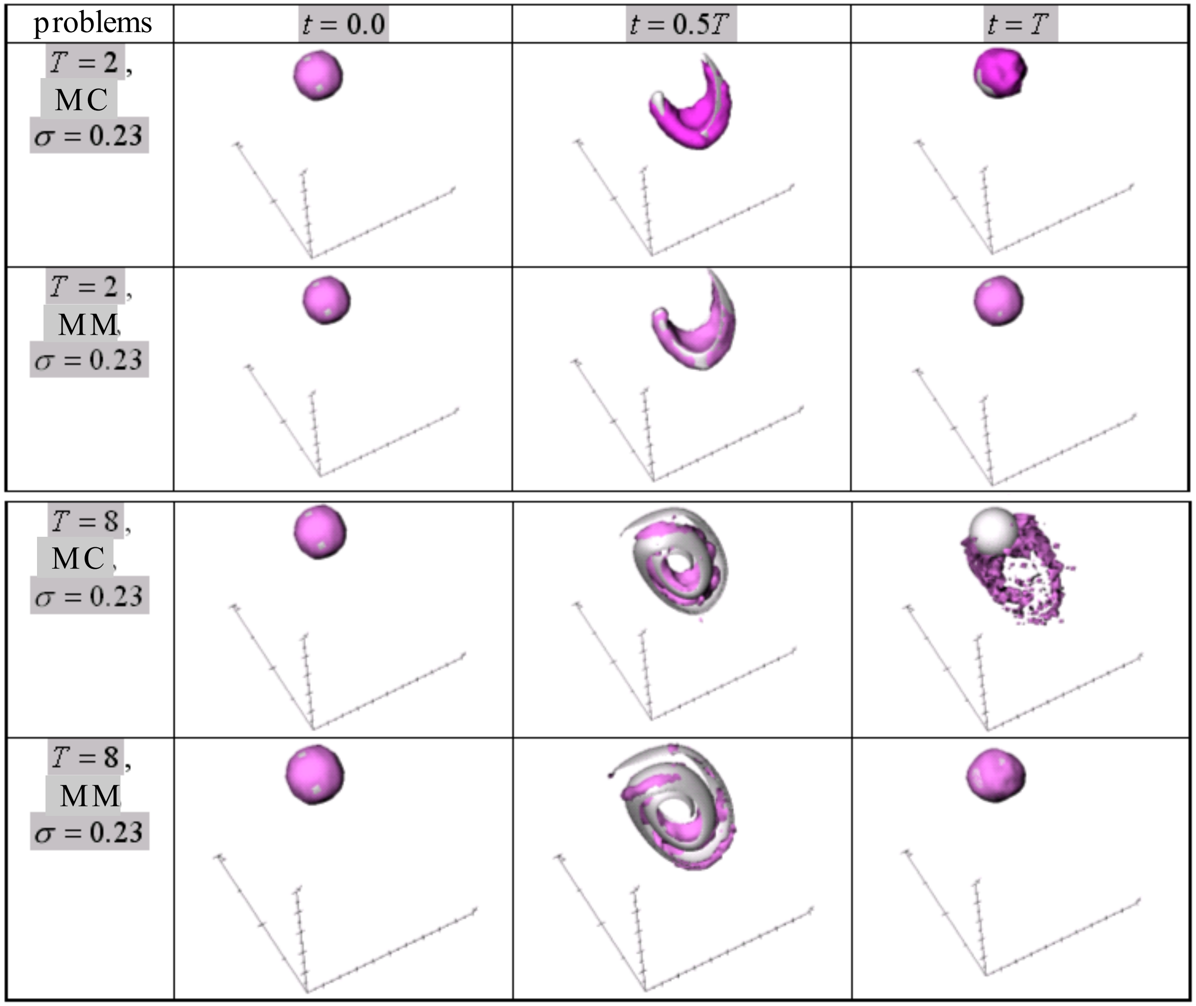
1. Incompressibility condition holds:

$$\partial u/\partial x + \partial v/\partial y + \partial w/\partial z = 0$$

2. No motion on boundaries (velocity components are zero)

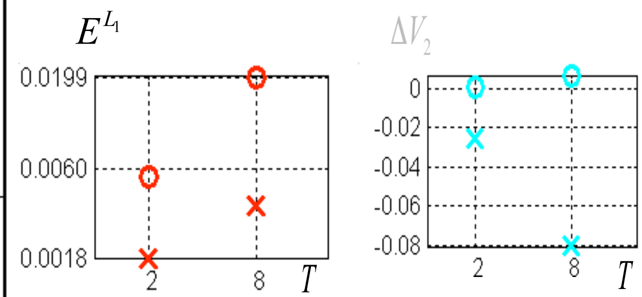
3. The system returns to the initial state at $t = T$

Time-reversible 3D flow with period T



The isosurface (dark red) obtained for $\sigma = 0.23$, and contact surfaces (grey) at different times; the sphere in the time-reversed flow with period T; MC - concentrations; MM - markers

Errors in 3D calculations at $t=T$:
O - concentrations
X - markers



Conclusion

— **The marker method requires more resources, increasing the time of calculation (<20%) .**

+ **The marker method provides more accurate interface reconstruction (the requirement of <u>symmetry is met</u>).**

+ **The marker method tracks volumes more accurately.**

= **Both the methods agree and give good results**